LA-UR-14-26966
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Title: Increased Efficiency and Functionality Inside the Moment-Based Accelerated Thermal Radiation Transport Algorithm

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Intended for: Talk at Oak Ridge National Laboratory

Issued: 2014-09-05

Increased Efficiency and Functionality Inside the Moment-Based Accelerated Thermal Radiation Transport Algorithm

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September 11, 2014

Problem Statement

We are interested in solving the thermal radiative transfer (TRT) equation,

$$\frac{1}{c}\frac{\partial I}{\partial t} + \hat{\Omega} \cdot \nabla I + \sigma I = \frac{\sigma a c T^4}{4\pi}, \tag{1}$$

in which

- $I = I(\vec{r}, \hat{\Omega}, t)$
- $\sigma = \sigma(T)$

and the material temperature is governed by the following ODE,

$$\rho C_v \frac{dT}{dt} - \int_{4\pi} d\hat{\Omega}(\sigma I - \frac{\sigma a c T^4}{4\pi}) = 0. \tag{2}$$

Source Iteration

One could attempt to solve this problem using *source iteration*,

$$\frac{I^{n+1,k} - I^n}{c\Delta t} + \hat{\Omega} \cdot \nabla I^{n+1,k} + \sigma I^{n+1,k} = \frac{\sigma ac \left(T^{n+1,k-1}\right)^4}{4\pi},$$

$$\rho C_v \frac{T^{n+1,k} - T^n}{\Delta t} - \int_{4\pi} d\hat{\Omega} \left(\sigma I^{n+1,k} - \frac{\sigma ac \left(T^{n+1,k}\right)^4}{4\pi} \right) = 0.$$

- This iteration is highly nonlinear and may converge very slowly.
- The process of obtaining $I^{n+1,k}$ in Eq. 3 is called a *transport sweep* and is a significant computational cost in any TRT algorithm.

Previous Work

Advanced algorithms have been designed in recent years which utilize *Moment-Based Acceleration*:

1. D.A. Knoll, Kord Smith, and H. Park. *Application of the Jacobian-Free Newton-Krylov method to nonlinear acceleration of transport source iteration in slab geometry*, Nuclear Science and Engineering, 167(2):122-132, February 2011.
2. H. Park, D. A. Knoll, R. M. Rauenzahn, C. K. Newman, J. D. Densmore and A. B. Wollaber, *An Efficient and Time Accurate, Moment-Based Scale-Bridging Algorithm for Thermal Radiative Transfer Problems*, SIAM J. Sci. Comput. 35(5), S18-S41, 2013
3. H. Park, J. D. Densmore, A. B. Wollaber, D. A. Knoll, and R. M. Rauenzahn, *Monte Carlo Solution Methods in a Moment-Based Scale-Bridging Algorithm for Thermal Radiative Transfer Problems: Comparison with Fleck and Cummings*, International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering, Sun Valley, ID, May 5 - 9, 2013.

Moment-Based Acceleration

We construct a "low-order" system of moment equations to accelerate the solution to the transport equation.

This yields the following advantages:

1. Algorithmic acceleration - For the 1-D Gray Marshak wave problem (discussed later) this yields a 13$\times$ reduction in the number of transport sweeps.
2. Tight multiphysics coupling via the low-order system - multiple kinetic models can interact via the low-order system.
3. These algorithms map well to future computing architectures.

Moment-Based Acceleration

We begin with the time-discretized transport equation,

$$\frac{I^{n+1} - I^n}{c\Delta t} + \hat{\Omega} \cdot \nabla I^{n+1} + \sigma I^{n+1} = \frac{\sigma a c \left(T^{n+1}\right)^4}{4\pi}, \tag{3}$$

and compute the 0^{th} and 1^{st} angular moments:

$$\frac{E^{n+1} - E^n}{\Delta t} + \nabla \cdot F^{n+1} + c\sigma E^{n+1} = \sigma a c \left(T^{n+1}\right)^4, \tag{4}$$

$$\frac{F^{n+1} - F^n}{c\Delta t} + \nabla \cdot \mathcal{E} c E^{n+1} + \sigma F^{n+1} = 0, \tag{5}$$

Definitions

$$\frac{E^{n+1} - E^n}{\Delta t} + \nabla \cdot F^{n+1} + c\sigma E^{n+1} = \sigma ac \left(T^{n+1}\right)^4, \tag{6}$$

$$\frac{F^{n+1} - F^n}{c\Delta t} + \nabla \cdot \mathcal{E} c E^{n+1} + \sigma F^{n+1} = 0, \tag{7}$$

In Eqs. 6 and 7 we have used several new terms:

$$E = \frac{1}{c} \int_{4\pi} d\hat{\Omega}\ I \tag{8}$$

$$F = \int_{4\pi} d\hat{\Omega}\ \hat{\Omega} I \tag{9}$$

$$\mathcal{E} = \frac{\int_{4\pi} d\hat{\Omega}\ \hat{\Omega}\hat{\Omega} I}{\int_{4\pi} d\hat{\Omega}\ I} \tag{10}$$

Low-Order System

We now define our Low-Order (LO) system

$$\frac{E^{n+1}-E^n}{\Delta t}+\nabla\cdot F^{n+1}+c\sigma E^{n+1}=\sigma ac\left(T^{n+1}\right)^4, \tag{11}$$

$$\frac{F^{n+1}-F^n}{c\Delta t}+\nabla\frac{c}{3}E^{n+1}+\sigma F^{n+1}=\gamma cE^{n+1}, \tag{12}$$

$$\rho C_v\frac{T^{n+1}-T^n}{\Delta t}-c\sigma E^{n+1}+\sigma ac\left(T^{n+1}\right)^4=0 \tag{13}$$

in which $\nabla\mathcal{E}cE$ has been replaced by an NDA[1]-like approximation:

$$\nabla\cdot\mathcal{E}cE=\nabla\frac{c}{3}E-\gamma cE \tag{14}$$

γ is referred to as the *consistency term*. γ accounts for transport effects and HO-LO truncation error mismatch.

[1] See *Application of the Jacobian-Free Newton-Krylov method to nonlinear acceleration of transport source iteration in slab geometry* by Knoll et al.

Predictor-Corrector Algorithm

We compute E^{n+1}, F^{n+1} and T^{n+1} using a predictor-corrector time-stepping scheme:

1. Predict: Solve LO System for approximation to T^{n+1}, T^* with γ and σ lagged from previous time-step.
2. Update opacity σ using T^*.
3. Using T^*, execute a single transport sweep for I^{n+1}.
4. Given I^{n+1}, compute E^{HO} and F^{HO}.
5. Compute new consistency term γ using E^{HO} and F^{HO}.
6. Correct: Solve LO System for E^{n+1}, F^{n+1} and T^{n+1} using current γ and σ.

Predictor-Corrector Algorithm

- In practice we find that the Predictor-Corrector algorithm is sufficient for gray (single frequency group) problems.
  - At each timestep, we find that $E^{HO} \approx E^{n+1}$. This is referred to as "consistency."
  - Using a Crank-Nicolson time-differencing scheme, this method was shown to be second-order accurate in time.
- For multifrequency problem, iteration between the transport sweep and the corrector step is often required to ensure consistency.

Solutions to the Low-Order System

Low-Order Solutions

The LO system needs to be solved (at least) twice per time-step:

$$\frac{E^{n+1} - E^n}{\Delta t} + \nabla \cdot F^{n+1} + c\sigma E^{n+1} = \sigma ac \left(T^{n+1}\right)^4, \tag{15}$$

$$\frac{F^{n+1} - F^n}{c\Delta t} + \nabla \frac{c}{3} E^{n+1} + \sigma F^{n+1} = \gamma c E^{n+1}, \tag{16}$$

$$\rho C_v \frac{T^{n+1} - T^n}{\Delta t} - c\sigma E^{n+1} + \sigma ac \left(T^{n+1}\right)^4 = 0 \tag{17}$$

- We could define a nonlinear equation, $\mathcal{G}(E, F, T) = 0$, which corresponds to the solution of the low-order equation, however this function can be very highly dimensional.
- Instead, we will write a nonlinear equation, $\mathcal{F}(E) = 0$, which has the same solution, in which F and T have been nonlinearly eliminated.

Nonlinear Elimination

Given E, we can compute F^{n+1} and T^{n+1} by solving the following two equations for F^{n+1} and T^{n+1} respectively:

$$\frac{F^{n+1} - F^n}{c\Delta t} + \nabla \frac{c}{3} E + \sigma F^{n+1} = \gamma c E, \tag{18}$$

$$\rho C_v \frac{T^{n+1} - T^n}{\Delta t} - c\sigma E + \sigma a c \left(T^{n+1}\right)^4 = 0 \tag{19}$$

Then, we can write $\mathcal{F}$ as a function of E,

$$\mathcal{F}(E) = \frac{E - E^n}{\Delta t} + \nabla \cdot F^{n+1}(E) + c\sigma E - \sigma a c \left(T^{n+1}(E)\right)^4.$$

$\mathcal{F}$ has fewer degrees of freedom, however the evaluation becomes slightly more complicated.

Solving $\mathcal{F}(E) = 0$

Traditionally, we have solved $\mathcal{F}(E) = 0$ via a Jacobian-Free Newton-Krylov method.

- GMRES is used to solve $J\delta E = -\mathcal{F}$.
- The Jacobian-vector product is approximated using a finite-difference:

$$Jv \approx \frac{\mathcal{F}(E + \epsilon v) - \mathcal{F}(E)}{\epsilon}$$

In our experience, this works well when

1. solving a gray HO problem (i.e. $I(\vec{r}, \hat{\Omega}, \nu, t) = I(\vec{r}, \hat{\Omega}, t)$)
2. σ is fixed throughout the solution to the LO system.

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2. σ is fixed throughout the solution to the LO system.

Trouble with JFNK

Suppose σ is a function of T^{n+1} inside the LO system. Now, we must solve

$$\rho C_v \frac{T^{n+1}(E) - T^n}{\Delta t} - c\sigma\left(T^{n+1}(E)\right) E + \sigma\left(T^{n+1}(E)\right) ac \left(T^{n+1}(E)\right)^4 = 0$$

1. Finite-difference Jacobian can be very inaccurate.
   - Choose the appropriate value for ϵ is challenging. E can vary by more than 10 orders of magnitude throughout the domain.
   - σ is often a highly nonlinear function of T and at times may be computed via table-lookup.
2. Analytic Jacobian-vector product becomes challenging when σ is a function of E.

Possible solution: Pick a method which does not need a Jacobian.

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Possible solution: Pick a method which does not need a Jacobian.

NKA as LO Solver

We will consider using Nonlinear Krylov Acceleration[2], a variant of Anderson Acceleration, as the LO Solver.

NKA is a nonlinear solver which

1. does not require an approximation to the Jacobian.
2. uses a history of residual evaluations to compute an update for the current iterate.

[2] see *Nonlinear Krylov Acceleration Applied to a Discrete Ordinates Formulation of the k-Eigenvalue problem* by Calef et al.

NKA as LO Solver

Nonlinear Krylov Acceleration

Input initial iterate x_0, history length M
Set $x_1 = x_0 - \mathcal{F}(x_0)$, $n = 1$.
while $\mathcal{F}(x_n) >$ tolerance **do**
Compute NKA Update

$$\vec{v}_{n+1} = \sum_{i=n-M+1}^{n} z_i^{(n)} \vec{v}_i + \left(\mathcal{F}(x_n) - \sum_{i=n-M+1}^{n} z_i^{(n)} \vec{w}_i \right)$$

in which

$$\vec{v}_i = x_{i-1} - x_i, \qquad \vec{w}_i = \mathcal{F}(x_{i-1}) - \mathcal{F}(x_i), \quad \vec{z}^{(n)} = \arg\min_{y \in \mathbb{R}^M} \left\| \mathcal{F}(x_n) - \sum_{i=n-M+1}^{m} y_i \vec{w}_i \right\|$$

Set $x_{n+1} = x_n + \vec{v}_{n+1}$.
Increment $n = n + 1$.
end while

Test Problems

- We will compare JFNK and NKA on two test problems:
  1. Two Material Problem
  2. Gray Marshak Wave
- For each problem, we will report the total number of low-order function evaluations.
- We use a Trilinos multi-level method to invert the preconditioner.
- We use a LDG spatial discretization and an S_n angular discretization.

Two-Material Problem

Properties:

- 1 cm domain with 100 uniform spatial cells.
- $\Delta t = 10^{-10}$ s for 500 time-steps.
- Problem is initially in equilibrium at 50 eV.
- At $t = 0$ a 500 eV isotropic source is applied at the left boundary.

Material Properties for 1-D 2 Material Problem

	Material 1	Material 2
x - range	< 0.5 cm	> 0.5 cm
σ (cm^{-1})	0.2	2000
ρ ($\mathrm{g/cm}^3$)	0.01	10.0
C_v (erg/eV-g)	10^{12}	10^{12}

Two-Material Problem Results

Method	LO Function Evals	LO Function Evals per Solve
NKA(3)	5473	5.473
NKA(5)	5466	5.466
NKA(7)	5466	5.466
JFNK	15618	15.618

For the purposes of comparison, we were able to compute the analytic Jacobian for this problem and use a direct inversion to compute the Newton step. In this case, 2944 function evaluations were required.

Results from 2014 Copper Mountain Conference on Iterative Methods.

Gray Marshak Wave Problem

Properties:

- 2.0 cm domain with 40 uniform spatial cells
- $\Delta t \in [10^{-11}, 10^{-10}]$ for 515 time-steps.
- $\rho = 1.0\ g/cm^3$
- $C_v = 1.3784 \times 10^{11}\ erg/eV - g$.
- Problem is initially in equilibrium at 0.025 eV.
- At $t = 0$, a 150 eV isotropic source is applied to the left boundary.
- The opacity is given by

$$\sigma(T) = \frac{10^6 \rho}{T^3}.$$

Gray Marshak Wave Problem Problem Results

Method	LO Function Evals	LO Function Evals per Solve
NKA(3)	6599	6.407
NKA(5)	6558	6.367
NKA(7)	6558	6.367
JFNK	19019	18.465

For the purposes of comparison, we were able to compute the analytic Jacobian for this problem and use a direct inversion to compute the Newton step. In this case, 3880 function evaluations were required.

Results from 2014 Copper Mountain Conference on Iterative Methods.

Interpretation

1. These results confirm findings from a previous MATLAB implementation of the algorithm.
2. We expected NKA to be competitive with or outperform Newton's method for several reasons:
   - JFNK requires potentially inaccurate finite-difference Jacobian-vector product evaluations.
   - NKA relies only on function evaluations.
   - In our experience, NKA performs very well when the initial iterate is very near the solution, which is generally satisfied by our predictor-corrector algorithm.
3. We intend to further investigate the robustness of NKA by incorporating a line search.

Residual Monte Carlo

Predictor-Corrector Algorithm

We compute E^{n+1}, F^{n+1} and T^{n+1} using a predictor-corrector time-stepping scheme:

1. Predict: Solve LO System for approximation to T^{n+1}, T^* with γ and σ lagged from previous time-step.
2. Update opacity σ using T^*.
3. Using T^*, execute a single transport sweep for I^{n+1}.
4. Given I^{n+1}, compute E^{HO} and F^{HO}.
5. Compute new consistency term γ using E^{HO} and F^{HO}.
6. Correct: Solve LO System for E^{n+1}, F^{n+1} and T^{n+1} using current γ and σ.

Motivation

We often like to compute the transport sweep via Monte Carlo simulation, however,

- The stochastic noise from a Monte Carlo (MC) transport sweep can provide challenges for accuracy and may negatively impact low-order solver.
- Global solutions are necessary, however MC does not excel with this.
- Advanced high-order (HO) solvers can be applied in the HO-LO setting.

Theory

- The stochastic noise in a MC simulation is proportional to the magnitude of the source term.
- Solution to high-order system can often be well-approximated.
- We create a residual system of equations which yields smaller source terms and thus produces less stochastic noise.

History of RMC

"Residual" Monte Carlo algorithms have been proposed previously in several forms. What we have accomplished differs from previous work in many ways -

1. The approximate time-step solution, I^+, in our formulation can be chosen to accomplish desired objectives - e.g. remove volumetric source term.
2. Our formulation is greatly simplified by the HO-LO algorithm - RMC needs to solve a purely absorbing problem at each time-step.
3. Exponentially Convergent Monte Carlo (ECMC) (see Peterson, Morel, and Ragusa, 2013) requires mesh-adaptation in both space and angle. Our algorithm operates on a single mesh.

Current State of Methods

- A gray, time-discrete 1-D RMC method has been implemented and tested inside the prototype code.
- An article describing these results has been published in JCP:

  Jeffrey Willert and H. Park, "Residual Monte Carlo High-Order Solver for Moment-Based Accelerated Thermal Radiative Transfer Equations," *Journal of Computational Physics*, 276, pp. 405-421 2014.

- A gray, time-continuous 1-D RMC method has been implemented using flat cell sources.

Flat Source, Backward-Euler Time Discretization

We wish to solve

$$\frac{I^{n+1} - I^n}{c\Delta t} + \mu\frac{\partial I^{n+1}}{\partial x} + \sigma^{n+1} I^{n+1} = \frac{\sigma^{n+1} ac \left(T^{n+1}\right)^4}{2}. \quad (20)$$

Given some approximation $I^+ \approx I^{n+1}$, we define

$$\delta^{n+1} = I^{n+1} - I^+. \quad (21)$$

Now we solve

$$\frac{\delta^{n+1}}{c\Delta t} + \mu\frac{\partial \delta^{n+1}}{\partial x} + \sigma^{n+1}\delta^{n+1} = \frac{\sigma^{n+1} ac \left(T^{n+1}\right)^4}{2} - \frac{I^+ - I^n}{c\Delta t} - \mu\frac{\partial I^+}{\partial x} - \sigma^{n+1} I^+ \quad (22)$$

for the residual correction term, δ^{n+1}.

Residual Source Term

Old source term:

$$S_{SMC} = \frac{\sigma^{n+1} ac \left(T^{n+1}\right)^4}{2} + \frac{I^n}{c\Delta t} \tag{23}$$

New source term:

$$S_{RMC} = \frac{\sigma^{n+1} ac \left(T^{n+1}\right)^4}{2} - \frac{I^+ - I^n}{c\Delta t} - \mu \frac{\partial I^+}{\partial x} - \sigma^{n+1} I^+. \tag{24}$$

Red terms yield a volumetric ($x - \mu$ space) source term. Blue term yields a face-source (fixed points in x-space) for discontinuous I^+.

Choosing I^+

Mathematically speaking - any choice of I^+ will allow for the correct solution to the HO problem given enough Monte Carlo particles.

- A good choice of I^+ allows user to gain acceptable level of MC error with relatively few particles.
- A bad choice of I^+ may require more MC particles than SMC.

Key realization: We can zero out the volumetric source term with the choice of I^+, i.e.

$$0 = \frac{\sigma^{n+1} ac \left(T^{n+1}\right)^4}{2} - \frac{I^+ - I^n}{c\Delta t} - \sigma^{n+1} I^+ \tag{25}$$

$$I^+ = \left[\frac{\sigma^{n+1} ac \left(T^{n+1}\right)^4}{2} + \frac{I^n}{c\Delta t}\right] / \left(\frac{1}{c\Delta t} + \sigma^{n+1}\right) \tag{26}$$

This allows us to sample a lower-dimensional space, in turn yielding less stochastic noise.

RMC HO Solver

1. Compute I^{+}.
2. Build residual source term.
3. Simulate particle histories (each of which begins on a cell face).
4. Tally δ^{n+1} at cell centers and cell faces.
5. Recover I^{n+1}, E^{n+1}, and F^{n+1}.

Computational Results - Two-Material Problem

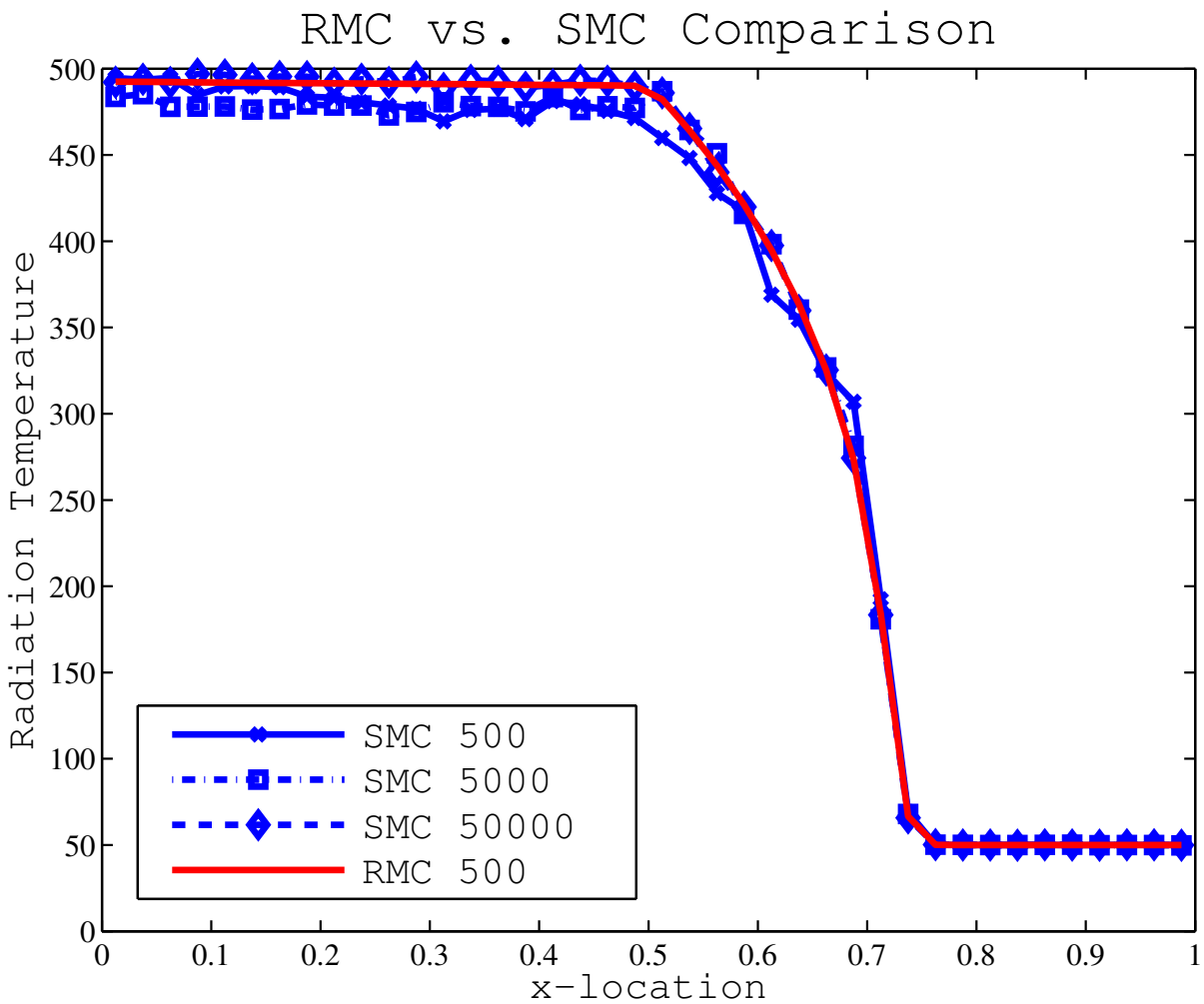
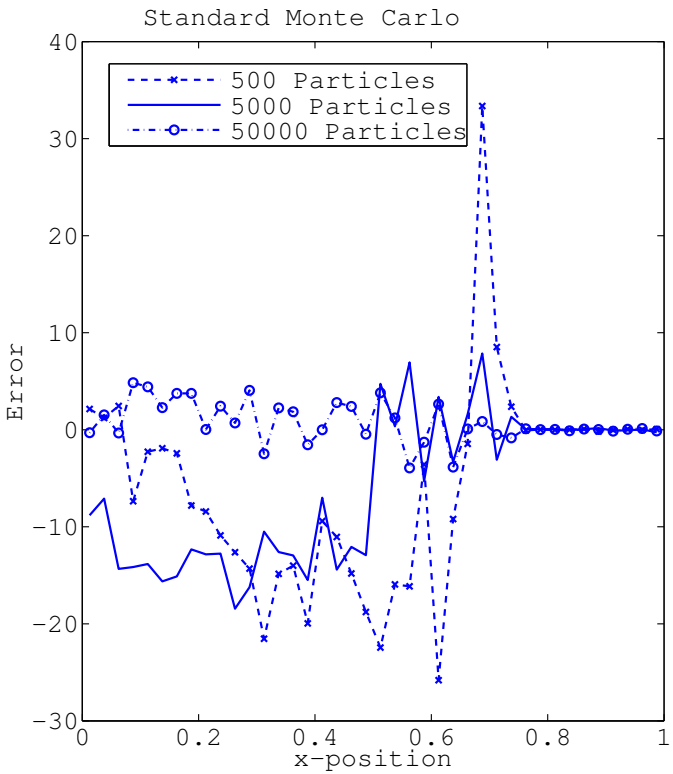
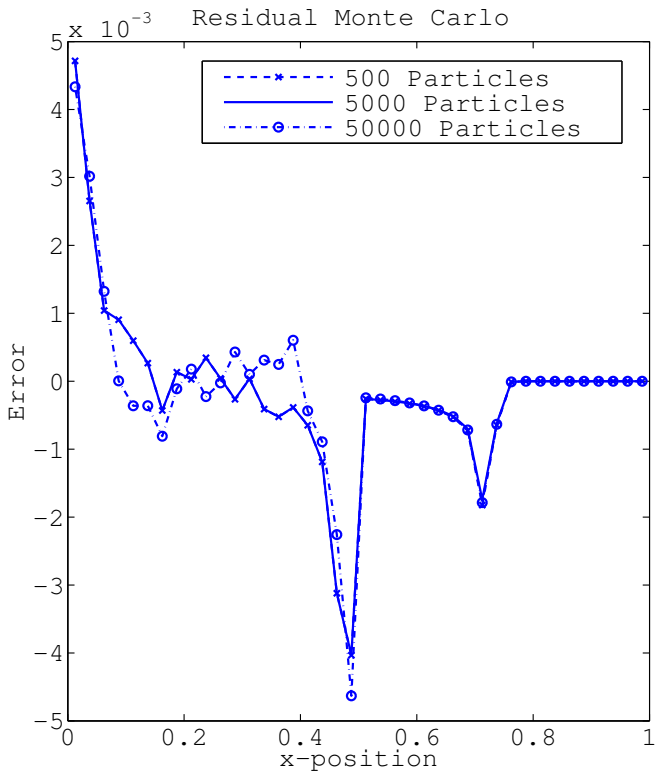


Figure: Comparison of SMC and RMC at $\Delta x = 0.025$ with 128 angular bins.

Computational Results - Two-Material Problem





RMC(500) demonstrates nearly zero stochastic noise, whereas SMC(50000) still exhibits significant errors.

Computational Results - Two-Material Problem

Table: Relative efficiency for Two-Material Problem using 40 Spatial Cells

Method	Particles	64 Bins	128 Bins
SMC	500	1	1
RMC	500	4917.8	6468.5
SMC	5000	1.734	0.498
RMC	5000	2450.4	4274.5
SMC	50000	0.462	0.313
RMC	50000	435.0	969.3

Relative efficiency measures (REMs) have been normalized so that SMC(500) has a REM $= 1$.

RMC(500) is roughly 20,000x more efficient than SMC(50,000).

Conclusions

1. The HOLO algorithm allows for a simple implementation of a residual Monte Carlo algorithm.
2. Careful choice of the approximating distribution, I^+, is required in order to minimize noise.
3. Stochastic noise can be minimized by placing particles in lower-dimensional spaces. For example, particles born on a cell-face generally contribute less noise than those born in the cell volume.
4. For time-discrete RMC, we have demonstrated relative efficiency measures varying between 500 and 12,000.
5. RMC incurs zero error in regions of the domain which remain in equilibrium, i.e. have zero spatial derivative.

Neutronics Applications

k-Eigenvalue problem

We are interested in solving the multi-group k-eigenvalue problem given by

$$\hat{\Omega} \cdot \nabla \psi_g(\hat{\Omega}, \vec{r}) + \Sigma_{t,g} \psi_g(\hat{\Omega}, \vec{r}) = \frac{1}{4\pi} \left[\sum_{g'=1}^{G} \Sigma_s^{g' \to g} \phi_{g'}(\vec{r}) + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \phi_{g'}(\vec{r}) \right]$$

k-Eigenvalue problem

As before, let us compute the zeroth angular moment of the transport equation

$$\nabla \cdot \vec{J}_g + \left(\Sigma_{t,g} - \Sigma_s^{g\to g}\right)\phi_g = \sum_{g'\neq g} \Sigma_s^{g'\to g}\phi_{g'} + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}\phi_{g'},$$

and then write $\vec{J}$ as

$$\vec{J}_g = -\frac{1}{3\Sigma_{t,g}}\nabla\phi_g + \hat{D}_g\phi_g.$$

This yields the following low-order system

$$\nabla \cdot \left[-\frac{1}{3\Sigma_{t,g}}\nabla\phi_g + \hat{D}_g\phi_g\right] + \left(\Sigma_{t,g} - \Sigma_s^{g\to g}\right)\phi_g = \sum_{g'\neq g} \Sigma_s^{g'\to g}\phi_{g'} + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}\phi_{g'}.$$

Note: $\hat{D}$ is the same as γ in the TRT HO-LO algorithm.

NDA-NCA

Compute initial iterate $\Phi^{(0)}$, initial eigenvalue approximation k^0. Set iteration counter $m = 0$.
while $|k^m - k^{m-1}| > \tau$ **do**
Update counter, $m = m + 1$.
Execute transport sweep and compute new consistency term

$$\Psi^{(m)} = \frac{1}{4\pi}\mathcal{L}^{-1}\left(\mathcal{S} + \frac{1}{k^{m-1}}\mathcal{F}\right)\Phi^{(m-1)}, \tag{27}$$

$$\Phi^{HO} = \int \Psi^{(m)} d\hat{\Omega}, \tag{28}$$

$$\vec{J}^{HO} = \int \hat{\Omega}\Psi^{(m)} d\hat{\Omega}, \tag{29}$$

$$\hat{D}^{(m)} = \frac{\vec{J}^{HO} + \frac{1}{3\Sigma_t}\nabla\Phi^{HO}}{\Phi^{HO}}. \tag{30}$$

Solve the LO eigenvalue problem for $\Phi^{(m)}$ and k^m

$$\left(\mathcal{D}^{(m)} - \mathcal{S}_U - \mathcal{S}_L\right)\Phi^{(m)} = \frac{1}{k^{(m)}}\mathcal{F}\Phi^{(m)}. \tag{31}$$

end while

NOTE: NDA-NCA achieves the *same eigenvalue and eigenvector as a purely high-order solver.* See references [1], [2], and [7].

Deterministic HO-LO Results[3] - 2D C5G7-MOX Problem

Method	Sweeps	Time (s)	HO Time (s)	LO Time (s)	Factor
NDA-NCA-JFNK	6	535.48	214.92	320.56	1.00
NDA-NCA-NKA	6	635.52	214.71	420.81	1.19
NDA-PI	13	2599.61	469.37	2130.24	4.85
HO-JFNK(.001,30)	179	6512.52	6512.52	—	12.16
HO-JFNK(.01,150)	154	5620.18	5620.18	—	10.50
HO-NKA(15)	121	4500.79	4500.79	—	8.41
PI(1)	1454	56387.71	56387.71	—	105.30
PI(10)	1970	72851.56	72851.56	—	136.05

Table key:

- PI(max) - Power Iteration (maximum number of inner iterations)
- HO-X - Nonlinear solver X is applied directly to high-order problem
- NDA-PI - Nonlinear Diffusion Accelerated calculation, low-order problem solved with power iterations
- NDA-NCA-X - Nonlinear Diffusion Accelerated calculation, low-order problem solved with nonlinear solver X

[3] see *A Comparison of Acceleration Methods for Solving the Neutron Transport k-Eigenvalue Problem* by Willert, Park and Knoll (JCP 2014)

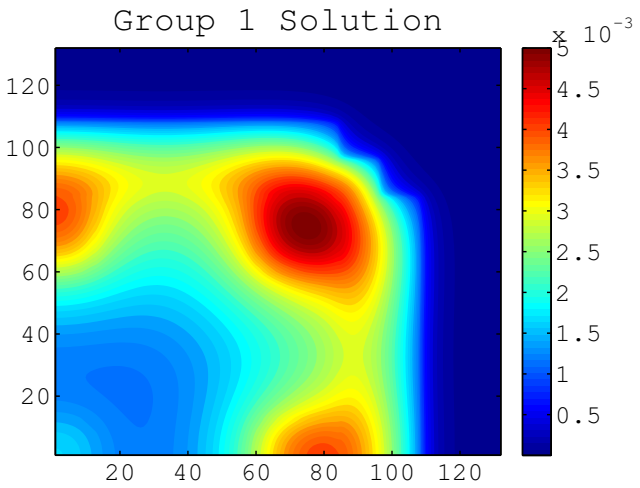
Hybrid HO-LO Method

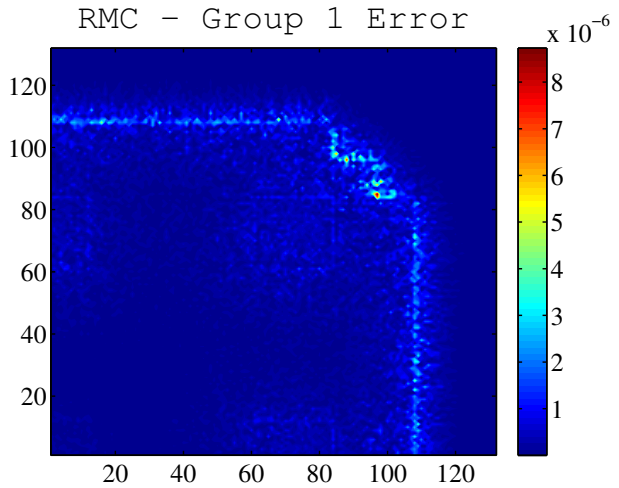
NDA-NCA has been adapted to use Monte Carlo simulation to replace the S_n transport sweep.[4]

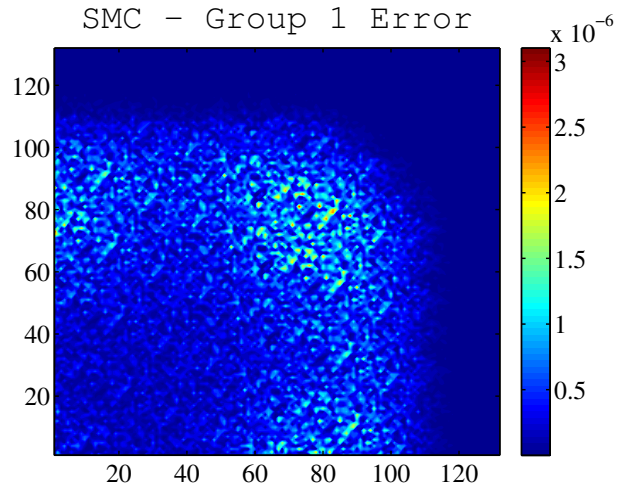
- To solve the 2-D, 2-group LRA-BWR problem required roughly 10^{11} particles to get 5 digits in the eigenvalue.
- Hybrid NDA-NCA is more efficient than analog Monte Carlo, but not by much.
- Can RMC help here?

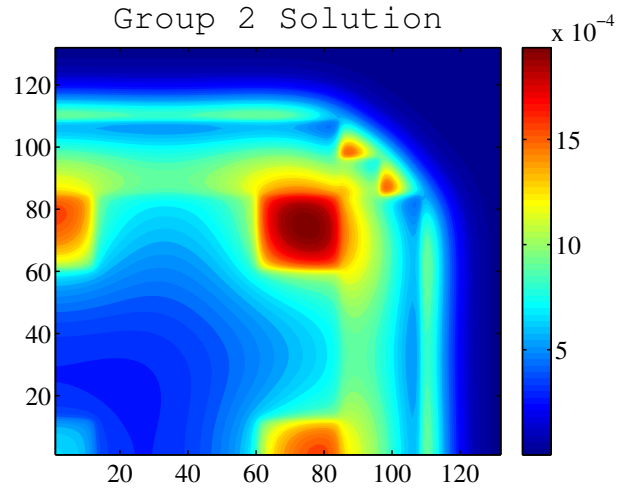
[4] see *A Hybrid Deterministic/Monte Carlo Method for Solving the k-Eigenvalue Problem with a Comparison to Analog Monte Carlo Solutions* by Willert, Kelley, Knoll and Park (Journal of Computational and Theoretical Transport)

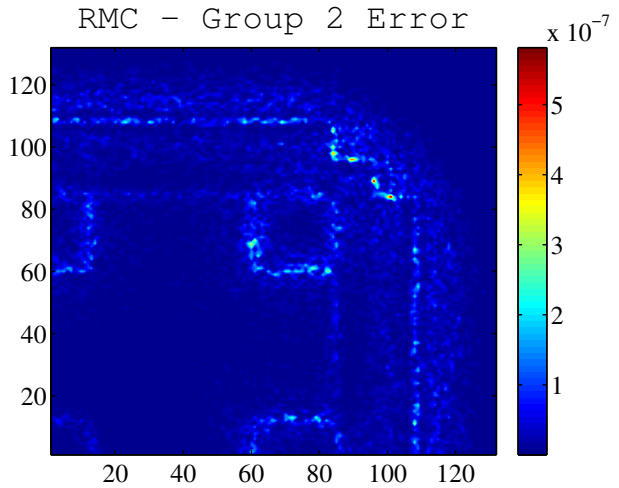
Neutronics RMC Results

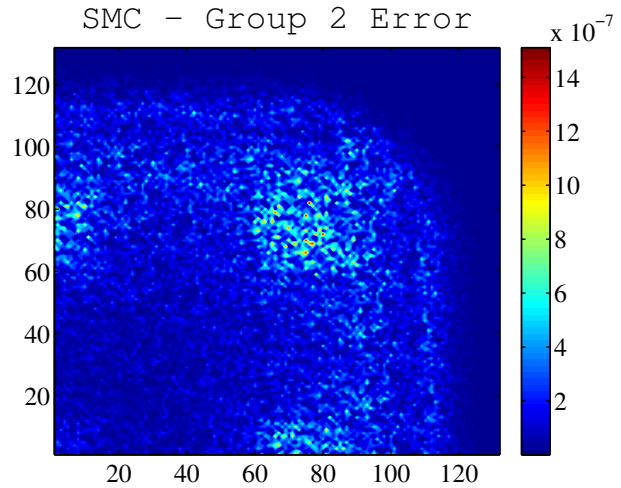












A similar accuracy solution is achieved by RMC for a factor of roughly 700 fewer particles.

Neutronics Conclusions

1. NDA-NCA has been shown to accelerate the solution to isotropic k-eigenvalue problems by a factor of over 100 compared to Power Iteration and a factor of over 10 for nonlinearly accelerated calculations.
2. Hybrid NDA-NCA can be accelerated by replacing a standard Monte Carlo simulation with "Residual Monte Carlo."
3. NDA-NCA has recently been adapted to accelerate anisotropic k-eigenvalue calculations.

(Subject of talk at ANS *Reactor Protection and Shielding Division* Conference in Knoxville, TN at 10:25 AM on 9/18)

Conclusions

1. We can now choose between JFNK and NKA for our low-order solver in both the TRT and neutronics applications.
   - For TRT, we see a 2 - 3$\times$ reduction in low-order function evaluations when NKA is used.
   - No significant difference was demonstrated between JFNK and NKA as the low-order solver in the neutronics application. The most significant improvement is seen by implementing a high-order/low-order accelerator.
2. Replacing Monte Carlo transport sweeps by Residual Monte Carlo can provide a dramatic gain in efficiency.
   1. For 1-D TRT, we see a factor of 500-12,000 gain in efficiency.
   2. For 2-D neutronics, a factor of 700 gain in efficiency has been demonstrated.

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Future Work

1. Optimize the Residual Monte Carlo algorithm for the neutronics problem.
2. Implement RMC in two spatial dimensions for the TRT problem.
3. Characterize the robustness of both JFNK and NKA for the TRT low-order problem when Monte Carlo returns noisy consistency terms.

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Questions?

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